

3-Ethyltoluene
620-14-4 | DTXSID6050386

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.78 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.53e-01

Confidence level: 7.62e-01

Nearest Neighbors from the Training Set

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Cyclohexyl acetate

Measured: 3.00

Predicted: 2.43

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3-Ethylhexane

Measured: 3.04

Predicted: 23.3

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Acetic acid, 2-nitrophenyl ester

Measured: 2.61

Predicted: 2.90e-03

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2,5-Dimethylphenol

Measured: 5.28e-01

Predicted: 6.38e-02

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Propane, 1-iodo-2-methyl-

Measured: 4.98e-01

Predicted: 12.6